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Electronic Structure Computation on a NUMA Parallel Supercomputer

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We investigate strategies for the optimal exploitation of a parallel computer consisting of clusters of shared-memory-parallel (SMP) nodes, using molecular electronic structure theory (triple-excitation component of many-body perturbation theory) as the example. Although inter-node communication must be handled using a message-passing paradigm, within the node more direct use of shared memory is possible. This leads naturally to the coding of hierarchical parallel algorithms, in which coarse-grained division of work between nodes (handled in our code by the the Global Arrays (GA) toolkit) encloses finer-grained parallel structures that can be conveniently programmed using OpenMP. An alternative strategy is to simply use GA in a single-level parallel implementation, and it is not clear from the outset whether this simpler approach is better or worse than the nested method. Comparative results on an 8-node 2-way-SMP IBM SP computer illustrate the relative performance of the two algorithms.